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THE Be-Si (BERYLLIUM-SILICON) SYSTEM

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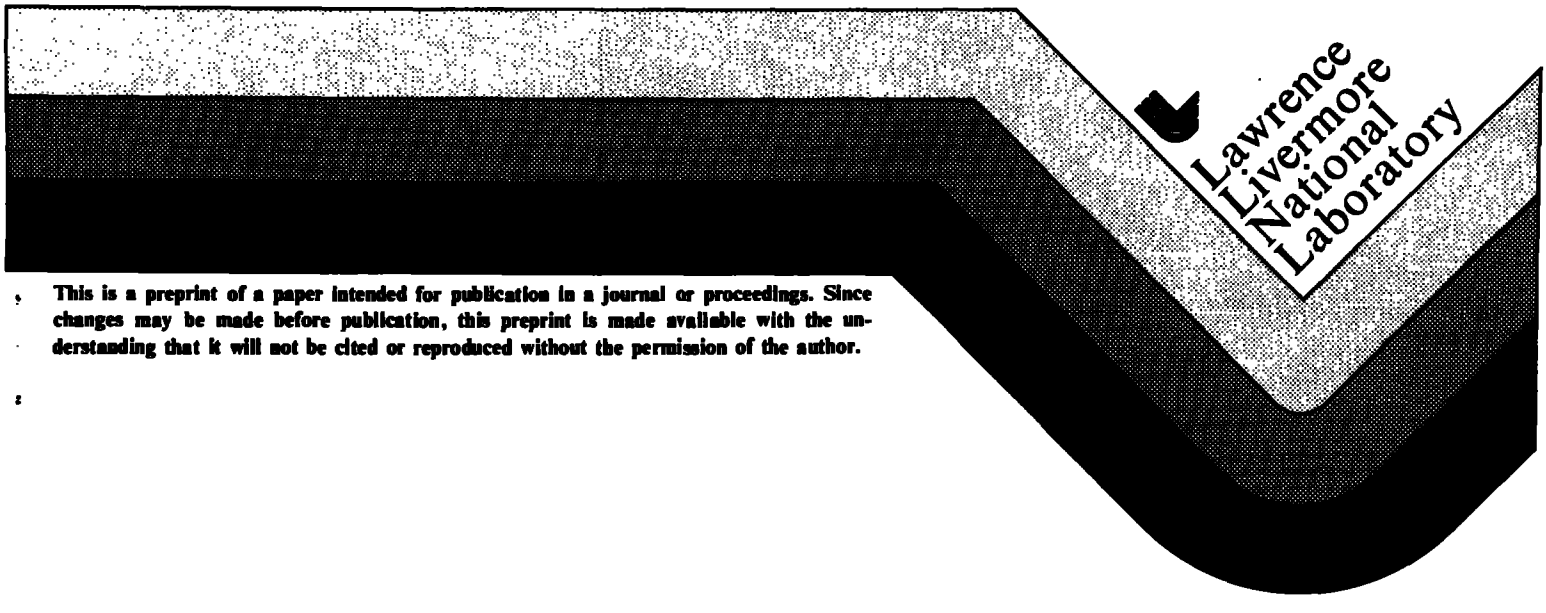

The Be-Si (Beryllium-Silicon) System

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Equilibrium Diagram

The assessed Be-Si phase diagram (Fig. 1) is based on the experimental work of [29Mas], who used only four specimens. The observed liquidus data do show a degree of uncertainty (see also [Hansen]). [46Ray] expected intermetallic compound formation based on the electronegativity of Si; however, the absence of intermediate phases has been confirmed by several investigators (e.g., [32Slo], [50Kau], [61Hin], [62Jor]). The solubility ranges of the terminal phases appear to be quite narrow.

(βBe) and (αBe) Terminal Solid Solutions. The melting point of βBe and the βBe --> αBe allotropic transformation temperature are 1289±4 and 1270±6 °C, respectively [85BAP]. Metallographic [32Slo, 50Kau] and X-ray lattice parameter [50Kau, 62Jor] studies did not reveal a solubility range for the (αBe) phase. [61Hin] observed that an alloy of 0.31 at.% Si was two-phase. Therefore, the solubility limit must be at least less than this value. Thermal analysis was not successful in defining the solubility limit of the (βBe) [61Gel].

(Si) Terminal Solid Solution. The melting point of Si is 1414 °C [Melt]. Solubility of Be in Si could not be detected by X-ray lattice parameter measurements [62Jor]. More recently, [82Tom] estimated the solid solubility of electrically active Be in (Si) from the resistivity profile of a diffusion couple. Solubility was expressed as $2.2\times10^{20}\exp(-1.97\times10^{4}/T)$ atoms/cm^3 for the temperature range between 800 and 1000 °C (or $0.402\exp(-1.97\times10^{4}/T)$ at.% assuming that the density of Si is 2.55 g/cm^3).

The lattice parameter changes in various alloys suggested the existence of some sizable solubility of Be in (Si) [61Jor1] or Si in (αBe) [61Jor2]. However, further detailed studies on rapidly quenched alloys did not reveal any solubility [62Jor].

L —> (αBe) + (Si) Eutectic Reaction. The liquidus and eutectic temperatures were measured by [29Mas].

Composition, at.% Si	Liquidus, °C	Eutectic, °C
0	1278	
7.4	1205	1065
24.3	1142	1090
42.8	1119	1090
64.5	1255	1088
100	1407	

The eutectic composition was proposed to be 33 at.% Si from the trend of arrest time with Si concentration at the eutectic temperature [29Mas]. [48Haj] redetermined the eutectic composition to be 38.5 at.% Si, presumably by reevaluating the liquidus trend due to [29Mas]). A best estimate based on the limited data is that the eutectic falls within the range 36±3 at.% Si.

Crystal Structures

A summary of crystal structure and lattice parameter data for pure elements is given in Table 1.

Thermodynamics

No experimental thermodynamic data are available. [78Bal] estimated the interaction parameter of liquid Be-Si by considering electronic and internal pressure effects. According to their regular solution and quasi-chemical models (Table 2), the calculated eutectic composition is displaced significantly toward Be-rich compositions (Fig. 2). The lattice stability parameters of Be and Si have been assumed (Table 2) from the heats of transformation given by [83Cha]. These may differ from the values used (but not given) by [78Bal]. The calculated diagram presented here is based on a subregular solution model and agrees slightly better with the experimental liquidus data. Further improvement of the modeling may be attained when the liquidus boundaries are better established through the use of purer materials and modern techniques.

[77Sud] calculated the activity of Si from the phase diagram given by [Hansen].

Table 1 Be-Si Crystal Structure and Lattice Parameter Data

Phase	Composition, at.% Si	Pearson symbol	Strukturbericht designation	Space group	Prototype	Lattice parameters, nm a	c	Reference
(βBe)....	0	cI2	A2	Im3m	W	0.25515	...	[King2]
(αBe)....	0	hP2	A3	$P6_3/mmc$	Mg	0.22857	0.35839	[King1]
(Si).....100		cF8	A4	Fd3m	diamond	0.54306	...	[King1]

Table 2 Thermodynamic Functions for the Be-Si System (J/mol)

Lattice Stability Parameters:

$G^{\circ}(Be,L) = 0$
$G^{\circ}(Si,L) = 0$
$G^{\circ}(Be,bcc) = -12600 + 8.067T$
$G^{\circ}(Be,cph) = -14700 + 9.428T$
$G^{\circ}(Si,diamond) = -50210 + 29.763T$

Excess Gibbs Energy of Mixing for the Liquid Phase:

$G^{ex} = 14916X(1-X)$ [78Bal] (Regular Solution Model)
$G^{ex} = 14916X(1-X)(1 - 449X(1-X)/T)$ [78Bal] (Quasi-Chemical Model)
$G^{ex} = X(1-X)(19142 -20027X)$ [Present] (Subregular Solution Model)

X: mole fraction of Si. T: Temperature in K.

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* Indicates key paper.
# Indicates presence of a phase diagram.

Be-Si Figure Captions

Fig. 1 Be-Si Assessed Phase Diagram

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Fig. 2 Comparison of Be-Si Assessed and Calculated Phase Boundaries

Thermodynamic models are given in Table 2.
——— = Assessed, ——— = Present model (Subregular),
— — — = [78Bal] (Regular), ——— = [78Bal] (Quasi-chemical).

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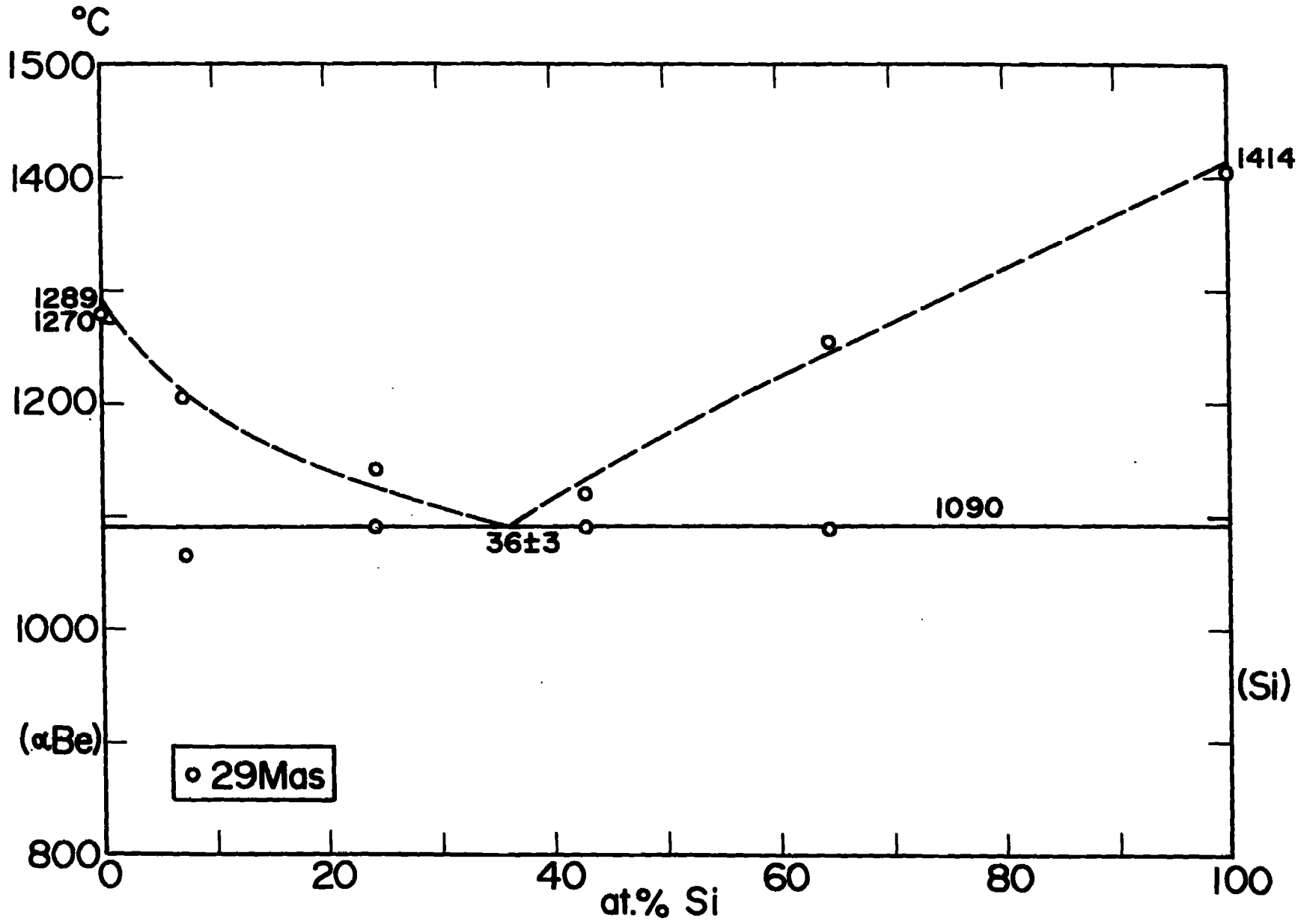
°C
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1400
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1270
1200
1414
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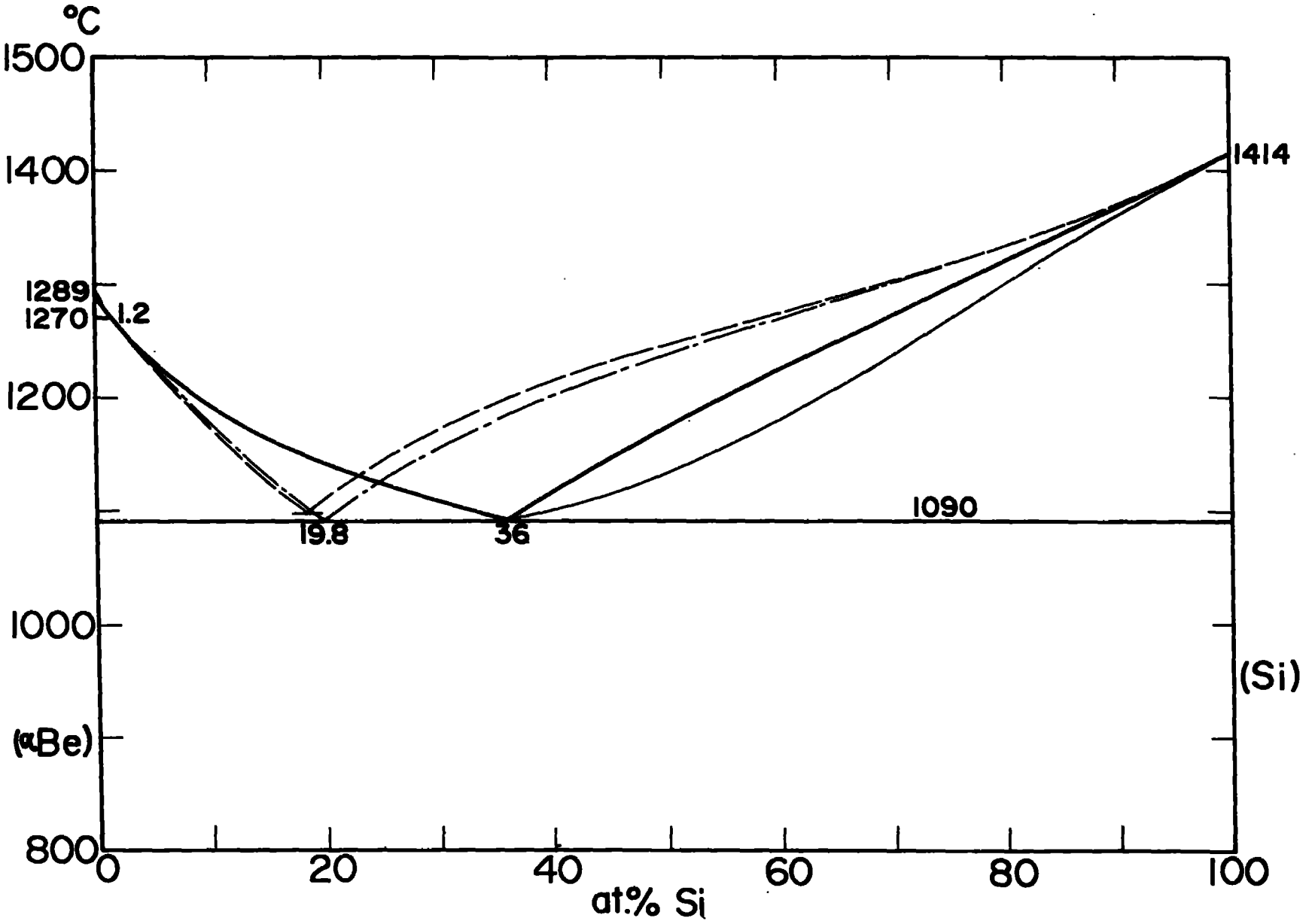
1000
(αBe)
(Si)
o 29Mas
800
0
20
40
60
80
100
at.% Si


°C
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1414
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19.8
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(αBe)
(Si)
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40
60
80
100
at.% Si